

# **Material Deposition at the Atomic and Molecular Level**

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# From the Molecular to the Macro Scale

## *Applications to the Semiconductor Industry*

*As feature sizes decrease, and new materials are explored, it becomes increasingly necessary to understand how interactions at the atomic and molecular scale manifest themselves as bulk material properties.*

### Difficult Challenges

- Model thin film and etch variation across die/wafer
- **Model new interconnect materials and interfaces**
- **Atomistic process modeling**

### Summary of Issues

*(being addressed by National Labs)*

- Reaction paths, rates, plasma models, equipment/feature scale links
- Atomistic simulation methods
- Grain structure, diffusion barriers
- Accurate models for process integration

***1999 Technology Roadmap for Semiconductors***

“Material properties and interfaces are well understood in the Al/SiO<sub>2</sub> system. Any change in materials will require that the new material and its interface be well characterized. New models based on adhesion science must be developed to allow detailed modeling under fabrication and use conditions ... .”

***1997 Report of the ad hoc Working Group on Interconnects***



**is a Three-Dimensional  
Feature-Scale Profile Simulator**

**Source Plane Models**

arbitrary energy and  
angular distribution functions

**Material transport**

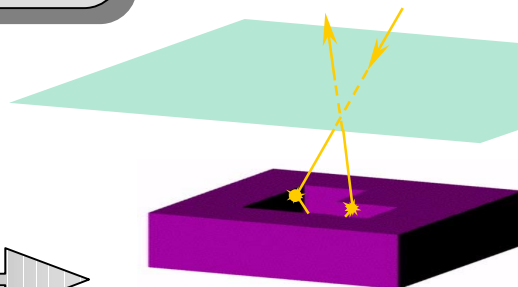
pressures/fluxes of gas phase species  
surface to surface visibility  
continuum or particle tracking

**Detailed Chemical Mechanisms**

CHEMKIN for gas phase chemistry  
SURFACE CHEMKIN for surface chemistry

**LaGriT -- 3D Wafer Geometry**

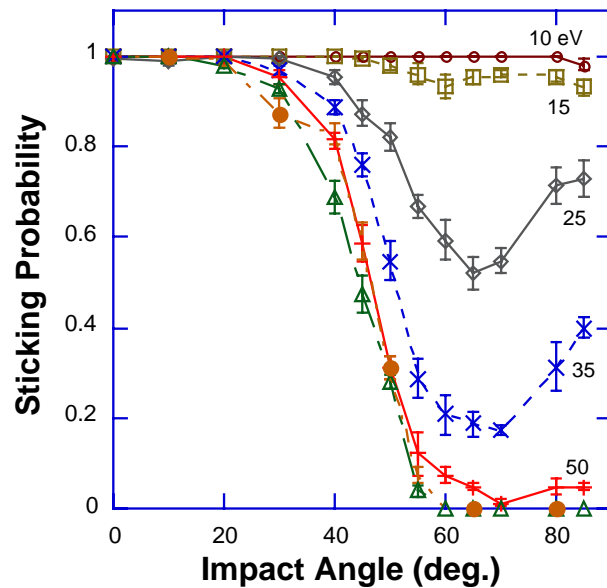
unstructured mesh, multiple materials  
adaptive refinement, smoothing, reconnect



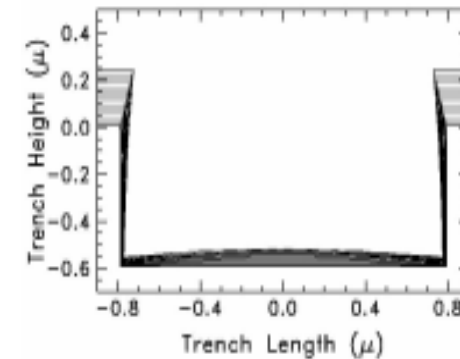
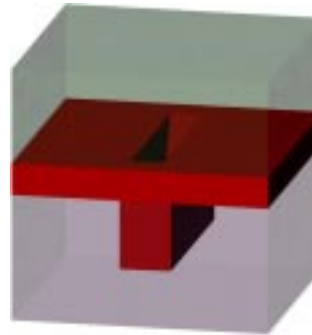


## Using Atomistic Simulation Data to Bridge Time and Length Scales

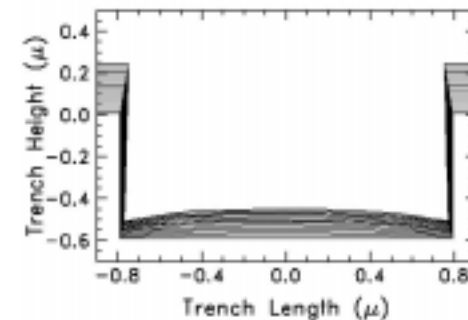
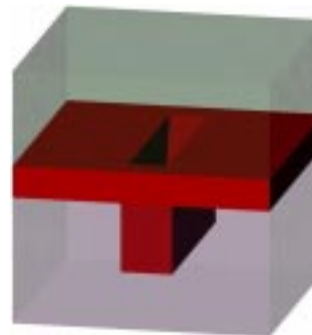
Use MD calculations  
to compute impact angle  
dependence of sticking probability



*constant sticking probability ( $s=1$ )*



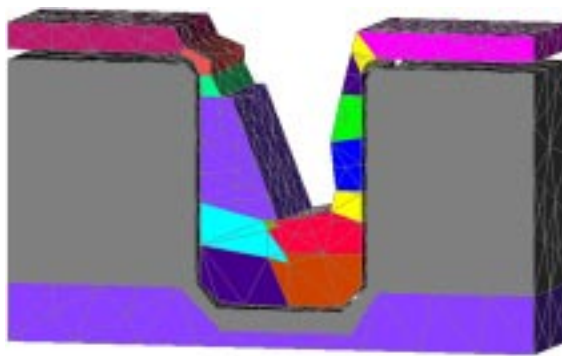
*atomistic sticking probability (at 50eV)*



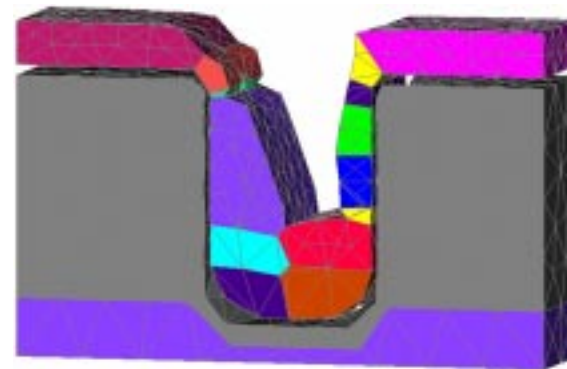


## Modeling Development of Microstructure

- Each grain a different material to SURFACE CHEMKIN and LaGriT
- TopoSim-3D and Grain3D exchange data through external files
  - TopoSim-3D generates triangle velocity vectors, pass to Grain3D
  - Grain3D advances time, generates new mesh object
- Images illustrate grain evolution during deposition



*time = 0*



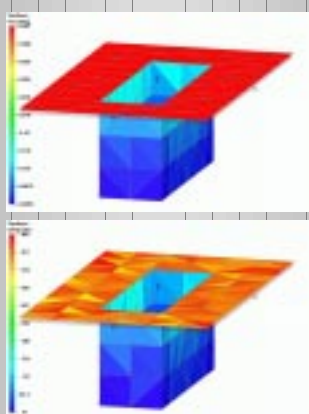
*time = 6 ms*



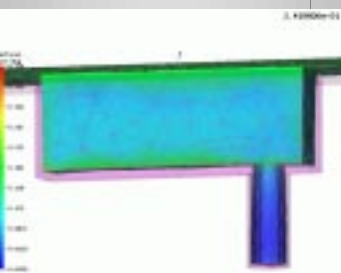
## Applications to Three-Dimensional Geometries

*Images shown display only the interfaces for several different 3D geometrical structures. Colors depict the local velocity of the interface -- red moves fastest, deep blue the slowest.*

continuum fluxes



particle fluxes



damascene geometry

Surface deposition rates can be modeled with continuum fluxes (above), or with Monte Carlo statistical methods using pseudo-particles (below). Both images are for the same physical system, a high surface reaction rate material, so growth rate at bottom of trench is much slower than on top.



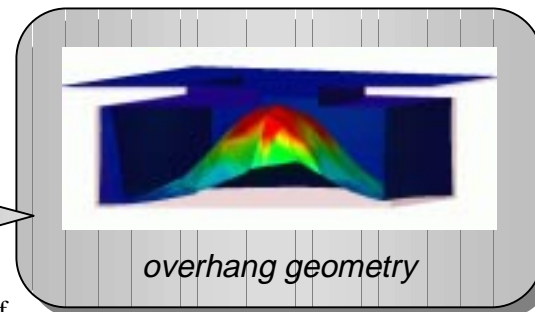
Image shows cutaway view of deposition into an overhang structure. The surface reaction rate is high, so little material deposits on walls or roof.



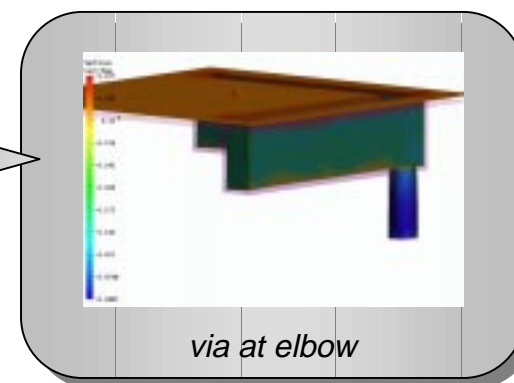
It would be difficult to achieve uniform step coverages using PVD methods for geometries such as shown here -- too poor a direct view from the source plane of *via* base.



Deposition with low growth rate material, shows that interface grows more uniformly, but slowest in the bottom of the *via* structure



overhang geometry



via at elbow

# Accelerated Molecular Dynamics (MD) of Thin Film Growth

## Problem: long time scales

- Deposition impact event is very quick ( $10^{-12}$  sec) -- use direct MD
- Time between deposition events is much longer ( $\geq 10^{-3}$  sec) -- diffusion processes important

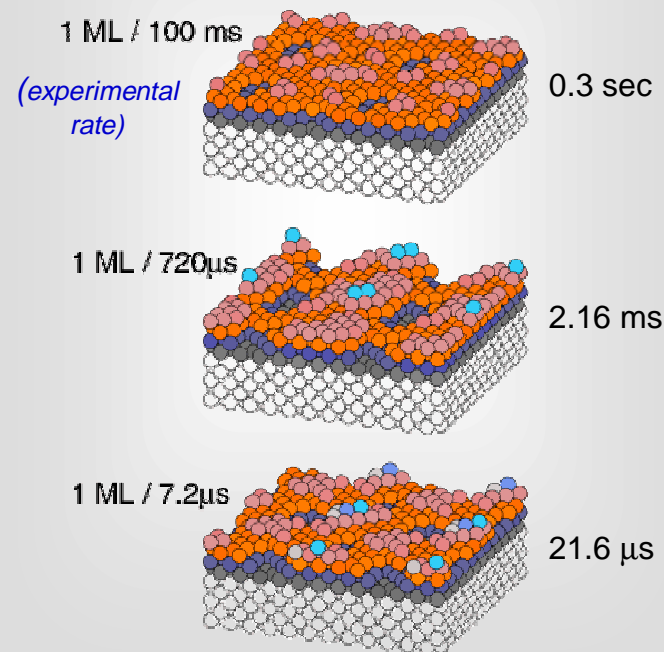
## Solution: Accelerated MD\* (Voter)

- Hyperdynamics = MD + Transition State Theory
- Parallel Replica Dynamics -- exploit parallelism to achieve longer time simulations

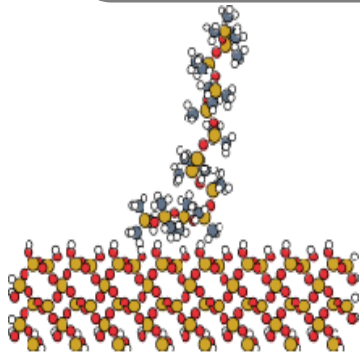
*\* supported by DOE Office of Basic Energy Sciences and Intel Corp (P. Leon)*

## Application:

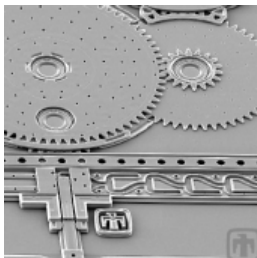
Cu/Cu(100) Thermal Deposition of 3 Monolayers (MLs) at  $T=100\text{K}$



## Ongoing Efforts at Los Alamos Can Be Adapted to Address New Interconnect Technologies



- Investigate properties of complex interfaces
  - *studies are currently underway on applying atomistic simulations to estimate the adhesion strength of polydimethylsiloxane on silica*
  - *continue development of nucleation models*



- Develop robust tools for bridging time and length scales
  - *continue development of plasma processes, etching*
  - *applications to corrosion processes*
  - *applications to electroplating*
  - *accelerated molecular dynamics*
  - *application to MEMS processes (in collaboration with Sandia National Laboratory)*